

Beyond Tonks-Girardeau: strongly correlated regime in quasi-one-dimensional Bose gases

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We consider a homogeneous 1D Bose gas with contact interactions and large attractive coupling constant. This system can be realized in tight waveguides by exploiting a confinement induced resonance of the effective 1D scattering amplitude. By using a variational *ansatz* for the many-body wavefunction, we show that for small densities the gas-like state is stable and the corresponding equation of state is well described by a gas of hard rods. By calculating the compressibility of the system, we provide an estimate of the critical density at which the gas-like state becomes unstable against cluster formation. Within the hard-rod model we calculate the one-body density matrix and the static structure factor of the gas. The results show that in this regime the system is more strongly correlated than a Tonks-Girardeau gas. The frequency of the lowest breathing mode for harmonically trapped systems is also discussed as a function of the interaction strength.

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The study of quasi-1D Bose gases in the quantum-degenerate regime has become a very active area of research. The role of correlations and of quantum fluctuations is greatly enhanced by the reduced dimensionality and 1D quantum gases constitute well suited systems to study beyond mean-field effects [1]. Among these, particularly intriguing is the fermionization of a 1D Bose gas in the strongly repulsive Tonks-Girardeau (TG) regime, where the system behaves as if it consisted of noninteracting spinless fermions [2]. The Bose-Fermi mapping of the TG gas is a peculiar aspect of the universal low-energy properties which are exhibited by bosonic and fermionic gapless 1D quantum systems and are described by the Luttinger liquid model [3]. The concept of Luttinger liquid plays a central role in condensed matter physics and the prospect of a clean testing for its physical implications using ultracold gases confined in highly elongated traps is fascinating [4, 5].

Bosonic gases in 1D configurations have been realized experimentally. Complete freezing of the transverse degrees of freedom and fully 1D kinematics has been reached for systems prepared in a deep 2D optical lattice [6, 7]. The strongly interacting regime has been achieved by adding a longitudinal periodic potential and the transition from a 1D superfluid to a Mott insulator has been observed [8]. A different technique to increase the strength of the interactions, which is largely employed in both bosonic and fermionic 3D systems [9] but has not yet been applied to 1D configurations, consists in the use of a Feshbach resonance. With this method one can tune the effective 1D coupling constant g_{1D} to essentially any value, including $\pm\infty$, by exploiting a confinement induced resonance [10]. For large and positive values of g_{1D} the system is a TG gas of point-like impenetrable bosons. On the contrary, if g_{1D} is large and negative, we will show that a new gas-like regime is en-

tered (super-Tonks) where the hard-core repulsion between particles becomes of finite range and correlations are stronger than in the TG regime. Some consequences of this new regime on the energetics of small systems in harmonic traps have already been pointed out in a preceding study [11]. In this Letter we investigate using Variational Monte Carlo (VMC) techniques the equation of state and the correlation functions of a homogeneous 1D Bose gas in the super-Tonks regime. We find that the particle-particle correlations decay faster than in the TG gas and that the static structure factor exhibits a pronounced peak. The momentum distribution and the structure factor of the gas are directly accessible in experiments by using, respectively, time-of-flight techniques and two-photon Bragg spectroscopy [8]. The study of collective modes also provides a useful experimental technique to investigate the role of interactions and beyond mean-field effects [6]. Within a local density approximation (LDA) for systems in harmonic traps we calculate the frequency of the lowest compressional mode as a function of the interaction strength in the crossover from the TG gas to the super-Tonks regime.

We consider a 1D system of N spinless bosons described by the following contact-interaction Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \frac{\partial^2}{\partial z_i^2} + g_{1D} \sum_{i<j} \delta(z_{ij}), \quad (1)$$

where m is the mass of the particles, $z_{ij} = z_i - z_j$ denotes the interparticle distance between particle i and j and g_{1D} is the coupling constant which we take large and negative. The study of the scattering problem of two particles in tight waveguides yields the following result for the effective 1D coupling constant g_{1D} in terms of

the 3D s -wave scattering length a_{3D} [10]

$$g_{1D} = -\frac{2\hbar^2}{ma_{1D}} = \frac{2\hbar^2 a_{3D}}{ma_{\perp}^2} \frac{1}{1 - Aa_{3D}/a_{\perp}}, \quad (2)$$

where $a_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$ is the characteristic length of the transverse harmonic confinement producing the waveguide and $A = |\zeta(1/2)|\sqrt{2} = 1.0326$, with $\zeta(\cdot)$ the Riemann zeta-function. The confinement induced resonance is located at the critical value $a_{3D}^c = a_{\perp}/A$ and corresponds to the abrupt change of g_{1D} from large positive values ($a_{3D} \lesssim a_{3D}^c$) to large negative values ($a_{3D} \gtrsim a_{3D}^c$). The renormalization (2) of the effective 1D coupling constant has been recently confirmed in a many-body calculation of Bose gases in highly elongated harmonic traps using quantum Monte Carlo techniques [11].

For positive g_{1D} , the Hamiltonian (1) corresponds to the Lieb-Liniger (LL) model. The ground state and excited states of the LL Hamiltonian have been studied in detail [12] and, in particular, the TG regime corresponds to the limit $g_{1D} = +\infty$. The ground state of the Hamiltonian (1) with $g_{1D} < 0$ has been investigated by McGuire [13] and one finds a soliton-like state with energy $E/N = -mg_{1D}^2(N^2 - 1)/24\hbar^2$. The lowest-lying gas-like state of the Hamiltonian (1) with $g_{1D} < 0$ corresponds to a highly-excited state that is stable if the gas parameter $na_{1D} \ll 1$, where n is the density and a_{1D} is the 1D effective scattering length defined in Eq. (2). This state can be realized in tight waveguides by crossing adiabatically the confinement induced resonance. The stability of the gas-like state can be understood from a simple estimate of the energy per particle. For a contact potential the interaction energy $E_{int}/N = g_{1D}n g_2(0)/2$ can be written in terms of the local two-body correlation function $g_2(0) = \langle \psi^\dagger(z)\psi^\dagger(z)\psi(z)\psi(z) \rangle / n^2$, where ψ^\dagger , ψ are the creation and annihilation particle operators. In the limit $g_{1D} \rightarrow -\infty$ one can use for the correlation function the result in the TG regime [14] $g_2(0) \simeq \pi^2 n^2 a_{1D}^2 / 3$, which does not depend on the sign of g_{1D} . In the same limit the kinetic energy can be estimated by $E_{kin}/N \simeq \pi^2 \hbar^2 n^2 / (6m)$, corresponding to the energy per particle of a TG gas. For the total energy $E = E_{kin} + E_{int}$ one finds the result $E/N \simeq \pi^2 \hbar^2 n^2 / (6m) - \pi^2 \hbar^2 n^3 a_{1D} / (3m)$, holding for $na_{1D} \ll 1$. For $na_{1D} < 0.25$ this equation of state yields a positive compressibility $mc^2 = n\partial\mu/\partial n$, where $\mu = dE/dN$ is the chemical potential and c is the speed of sound, corresponding to a stable gas-like phase. We will show that a more precise estimate gives that the gas-like state is stable against cluster formation for $na_{1D} \lesssim 0.35$.

The analysis of the gas-like equation of state is carried out using the VMC technique. The trial wavefunction employed in the calculation is of the form $\psi_T(z_1, \dots, z_N) = \prod_{i < j} f(z_{ij})$, where the two-body Jastrow term is chosen as

$$f(z) = \begin{cases} \cos[k(|z| - \bar{Z})] & \text{for } |z| \leq \bar{Z} \\ 1 & \text{for } |z| > \bar{Z} \end{cases} \quad (3)$$

The cut-off length \bar{Z} is a variational parameter, while the wave vector k for a given \bar{Z} is chosen such that the boundary condition at $z = 0$ imposed by the δ -function potential is satisfied: $-k \tan(k\bar{Z}) = 1/a_{1D}$. For distances smaller than the cut-off length, $|z| \leq \bar{Z}$, the above wave function corresponds to the exact solution with positive energy of the two-body problem with the interaction potential $g_{1D}\delta(z)$. For $g_{1D} < 0$ ($a_{1D} > 0$) the wavefunction $f(z)$ changes sign at a nodal point which, for $\bar{Z} \gg a_{1D}$, is located at $|z| = a_{1D}$. The variational energy is calculated through the expectation value of the Hamiltonian (1) on the trial wave function $E = \langle \psi_T | H | \psi_T \rangle / \langle \psi_T | \psi_T \rangle$. In the calculations we have used $N = 100$ particles with periodic boundary conditions and because of the negligible dependence of the variational energy on the parameter \bar{Z} we have used in all simulations the value $\bar{Z} = L/2$, where L is the size of the simulation box. Calculations carried out with larger values of N have shown negligible finite size effects.

The results for the variational energy as a function of the gas parameter na_{1D} are shown in Fig. 1 with solid symbols. For small values of the gas parameter our variational results agree very well with the equation of state of a gas of hard-rods (HR) of size a_{1D} (thick dashed line). The HR energy per particle can be calculated exactly from the energy of a TG gas by accounting for the excluded volume [2]

$$\frac{E_{HR}}{N} = \frac{\pi^2 \hbar^2 n^2}{6m} \frac{1}{(1 - na_{1D})^2}. \quad (4)$$

For larger values of na_{1D} , the variational energy increases with the gas parameter more slowly than in the HR case and deviations are clearly visible. By fitting a polynomial function to our variational results we obtain the best fit shown in Fig. 1 as a thick solid line. The compressibility obtained from the best fit is shown in Fig. 1 as a thin solid line and compared with mc^2 of a HR gas (thin dashed line). As a function of the gas parameter the compressibility shows a maximum and then drops abruptly to zero. The vanishing of the compressibility implies that the system is mechanically unstable against cluster formation. Our variational estimate yields $na_{1D} \simeq 0.35$ for the critical value of the density where the instability appears. This value coincides with the critical density for collapse calculated in the center of the trap for harmonically confined systems [11]. It is worth noticing that the VMC estimate of the energy of the system can be extended beyond the instability point, as shown in Fig. 1. This is possible since the finite size of the simulation box hinders the long-range density fluctuations that would break the homogeneity of the gas. This feature is analogous to the one observed in the quantum Monte-Carlo characterization of the spinodal point in liquid ^4He [15].

As shown in Fig. 1, the HR model describes accurately the equation of state for small values of the gas parameter. A similar accuracy is therefore expected for the correlation functions of the system. The correlation functions of a HR gas of size a_{1D} can be calculated from the

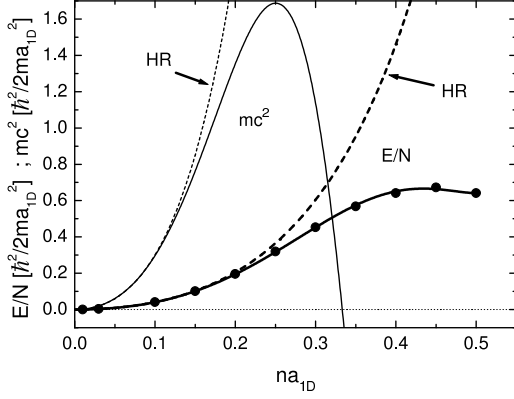


FIG. 1: Energy per particle and compressibility as a function of the gas parameter na_{1D} . Solid symbols and thick solid line: VMC results and polynomial best fit; thick dashed line: HR equation of state [Eq. (4)]. Thin solid and dashed line: compressibility from the best fit to the variational equation of state and from the HR equation of state respectively.

exact wave function [16] $\psi_{HR} = \prod_{i < j} |\sin[\pi(z'_i - z'_j)/L]|$, where the set of coordinates $\{z'_j\}$ is obtained from the set $\{z_j\}$ with the ordering $z_1 < z_2 - a_{1D} < z_3 - 2a_{1D} < \dots < z_N - (N-1)a_{1D}$ using the transformation $z'_j = z_j - ja_{1D}$, with $j = 1, 2, \dots, N$. We calculate the static structure factor $S(k)$, which in terms of the density fluctuation operator $\rho_k = \sum_{i=1}^N e^{ikz_i}$, is defined as

$$S(k) = \frac{1}{N} \frac{\langle \psi_{HR} | \rho_k \rho_{-k} | \psi_{HR} \rangle}{\langle \psi_{HR} | \psi_{HR} \rangle}, \quad (5)$$

and the one-body density matrix

$$g_1(z) = \frac{N}{n} \frac{\int \psi_{HR}^*(z_1 + z, \dots, z_N) \psi_{HR}(z_1, \dots, z_N) dz_2 \dots dz_N}{\int |\psi_{HR}(z_1, \dots, z_N)|^2 dz_1 \dots dz_N}. \quad (6)$$

Contrarily to the TG case, it is not possible to obtain analytical expressions for $g_1(z)$ and $S(k)$ in the HR problem. We have calculated them using configurations generated by a Monte Carlo simulation according to the exact probability distribution $|\psi_{HR}|^2$. The results for the static structure factor are shown in Fig. 2. Compared to $S(k)$ in the TG regime, a clear peak is visible for values of k of the order of twice the Fermi wave vector $k_F = \pi n$ and the peak is more pronounced as na_{1D} increases. The change of slope for small values of k reflects the increase of the speed of sound c with na_{1D} . The long-range behavior of $g_1(z)$ can be obtained from the hydrodynamic theory of low-energy excitations [17]. For $|z| \gg \xi$, where $\xi = \hbar/(\sqrt{2}mc)$ is the healing length of the system, one finds the following power-law decay

$$g_1(z) \propto 1/|z|^\alpha, \quad (7)$$

where the exponent α is given by $\alpha = mc/(2\pi\hbar n)$. For a TG gas $mc = \pi\hbar n$, and thus $\alpha_{TG} = 1/2$. For a HR gas

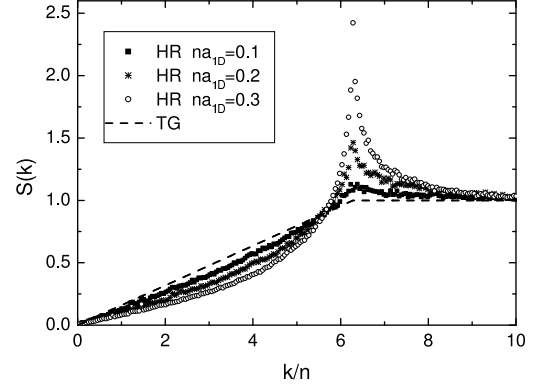


FIG. 2: Static structure factor $S(k)$ for a gas of HR at different values of the gas parameter na_{1D} (symbols) and for a TG gas (dashed line).

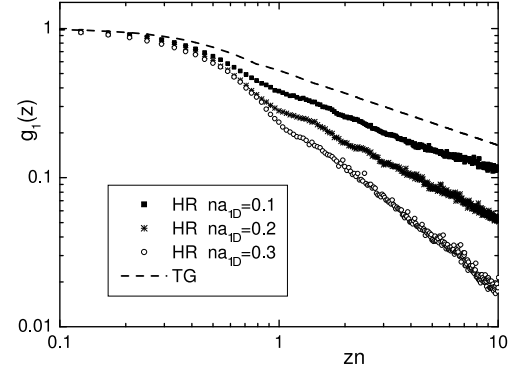


FIG. 3: One-body density matrix $g_1(z)$ for a gas of HR at different values of the gas parameter na_{1D} (symbols) and for a TG gas (dashed line).

one finds $\alpha = \alpha_{TG}/(1 - na_{1D})^2$ and thus $\alpha > \alpha_{TG}$. This behavior at long range is clearly shown in Fig. 3 where we compare $g_1(z)$ of a gas of HR with $na_{1D} = 0.1, 0.2$ and 0.3 to the result of a TG gas [18]. The long-range power-law decay of $g_1(z)$ is reflected in the infrared divergence of the momentum distribution $n(k) \propto 1/|k|^{1-\alpha}$ holding for $|k| \ll 1/\xi$. A gas of HR exhibits a weaker infrared divergence compared to a TG gas. The correlation functions of a HR gas at $na_{1D} = 0.1, 0.2$ should accurately describe the physical situation of a Bose gas with large and negative g_{1D} . For $na_{1D} = 0.3$ we expect already some deviations from the HR model, as it is evident from the equation of state in Fig. 1, which should broaden the peak in $S(k)$ and decrease the slope of the power-law decay in $g_1(z)$ at large distances. The analysis of correlation functions clearly shows that the super-Tonks regime corresponds to a Luttinger liquid where short range correlations are significantly stronger than in the TG gas.

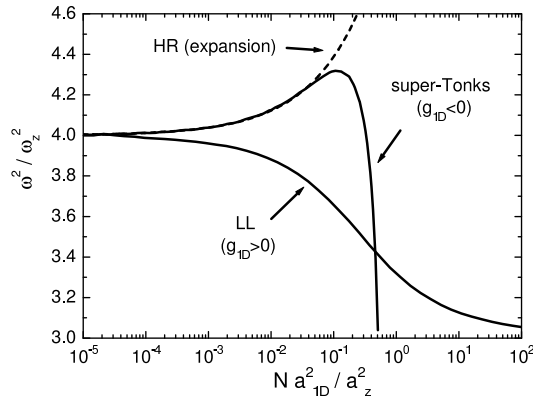


FIG. 4: Square of the lowest breathing mode frequency, ω^2 , as a function of the coupling strength Na_{1D}^2/a_z^2 for the LL Hamiltonian ($g_{1D} > 0$) and in the super-Tonks regime ($g_{1D} < 0$). The dashed line is obtained from the HR expansion (see text).

Another possible experimental signature of the super-Tonks regime can be provided by the study of collective modes. To this aim, we calculate the frequency of the lowest compressional mode of a system of N particles in a harmonic potential $V_{ext} = \sum_{i=1}^N m\omega_z^2 z_i^2/2$. We make use of LDA which allows us to calculate the chemical potential of the inhomogeneous system $\tilde{\mu}$ and the density profile $n(z)$ from the local equilibrium equation $\tilde{\mu} = \mu[n(z)] + m\omega_z^2 z^2/2$, and the normalization condition $N = \int_{-R}^R n(z) dz$, where $R = \sqrt{2\tilde{\mu}/(m\omega_z^2)}$ is the size of cloud. For densities n smaller than the critical density for cluster formation, $\mu[n]$ is the equation of state of the homogeneous system derived from the fit to the VMC energies (Fig. 1). From the knowledge of the density profile $n(z)$ one can obtain the mean square radius of the cloud $\langle z^2 \rangle = \int_{-R}^R n(z) z^2 dz / N$ and thus, making use of the result [19]

$$\omega^2 = -2 \frac{\langle z^2 \rangle}{d\langle z^2 \rangle / d\omega_z^2}, \quad (8)$$

one can calculate the frequency ω of the lowest breathing mode. Within LDA, the result will depend only on the dimensionless parameter Na_{1D}^2/a_z^2 , where $a_z = \sqrt{\hbar/m\omega_z}$ is the harmonic oscillator length. For $g_{1D} > 0$, i.e. in the case of the LL Hamiltonian, the frequency of the lowest compressional mode increases from $\omega = \sqrt{3}\omega_z$ in the weak-coupling mean-field regime ($Na_{1D}^2/a_z^2 \gg 1$) to $\omega = 2\omega_z$ in the strong-coupling TG regime ($Na_{1D}^2/a_z^2 \ll 1$). The results for ω in the super-Tonks regime are shown in Fig. 4 as a function of the coupling strength. In the regime $Na_{1D}^2/a_z^2 \ll 1$, where the HR model is appropriate, we can calculate analytically the first correction to the frequency of a TG gas. One finds the result $\omega = 2\omega_z[1 + (16\sqrt{2}/15\pi^2)(Na_{1D}^2/a_z^2)^{1/2} + \dots]$. Fig. 4 shows that this expansion accurately describes the frequency of the breathing mode when $Na_{1D}^2/a_z^2 \ll 1$, for larger values of the coupling strength the frequency reaches a maximum and drops to zero at $Na_{1D}^2/a_z^2 \simeq 0.6$. The observation of a breathing mode with a frequency larger than $2\omega_z$ would be a clear signature of the super-Tonks regime.

In conclusion we have pointed out the existence of a strongly correlated regime in quasi-1D Bose gases beyond the Tonks-Girardeau regime. This regime can be entered by exploiting a confinement induced resonance of the effective 1D scattering amplitude. We calculate the equation of state of the gas in the super-Tonks regime using VMC and we estimate the critical density for the onset of instability against cluster formation. The static structure factor and one-body density matrix are calculated exactly within the hard-rod model, which provides the correct description of the system for small values of the gas parameter. For harmonically trapped systems we provide explicit predictions for the frequency of the lowest compressional mode.

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